

Acetic acid, trifluoro-, methyl ester
431-47-0 | DTXSID2059988

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.95 | 0.69 | 0.95 | 0.65 | 0.96 | 0.68 |

Model Results

Predicted value: 1.63

Global applicability domain: Inside

Local applicability domain index: 9.75e-01

Confidence level: 6.16e-01

Nearest Neighbors from the Training Set

Image not found

Nitromethane

Measured: 2.53

Predicted: 1.63

Image not found

Propane

Measured: 0.97

Predicted: 1.60

Image not found

Dimethyl ether

Measured: 1.37

Predicted: 1.58

Image not found

Chloromethane

Measured: 1.39

Predicted: 1.58

Image not found

Methyl formate

Measured: 1.75

Predicted: 1.78